(P1-21)

Strong coupling between local electronic state and dynamical Jahn-Teller distortion at a vacancy in crystalline silicon

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Recently, Goto *et al.* [1] have discovered an anomalous softening of elastic constant below 10K in pure crystalline silicon, where the 3-fold degenerate ground state of a silicon vacancy is responsible for the softening. Early theoretical studies showed that the 3-fold degeneracy of the silicon vacancy state is removed due to the Jahn-Teller distortion [2]. It seems to be inconsistent with the newly observed experiment. However, the nonadiabatic effect of the distortion, which is considered to play crucial role at low temperature, was not considered there. We investigate the silicon vacancy state, paying attention to the effects of the nonadiabatic electron-phonon interaction and the electron correlation. To discuss these effects, we introduce a cluster model Hamiltonian:

$$\mathcal{H} = \sum_{i=1}^{6}\sum_{j=1}^{6}\sum_{\sigma=\pm1} t_{ij}(Q_x,Q_y,Q_z,Q_B)a_{i\sigma}^{\dagger}a_{j\sigma} + U\sum_{i=1}^{4} a_{i\uparrow}^{\dagger}a_{i\uparrow}a_{i\downarrow}^{\dagger}a_{i\downarrow}$$
$$+\frac{1}{2M_E}(P_x^2+P_y^2+P_z^2) + \frac{1}{2M_B}P_B^2 + \frac{1}{2}K_E(Q_x^2+Q_y^2+Q_z^2) + \frac{1}{2}K_BQ_B^2,$$

where $a_{i\sigma}^{\dagger}$ $(i=1-4)$ are creation operators of an electron with spin σ for 4 orbitals of dangling bond in a silicon vacancy and $a_{i\sigma}^{\dagger}$ $(i=5,6)$ are those for 2 orbitals representing the valence band and the conduction band, respectively. U is the Coulomb interaction and Q_x,Q_y,Q_z and Q_B are distortions for 3 tetragonal modes and a breathing mode, respectively. Within the adiabatic approximation for distortions together with the mean-field approximation for Coulomb interaction, this cluster model reproduces the early theoretical results [2]. By using the numerical diagonalization method for the cluster model, we take into account of both the nonadiabatic and the correlation effects, and find that the 3-fold degeneracy in the ground state is stable against the Jahn-Teller distortion due to strong quantum fluctuation which is caused by nonadiabatic electron-phonon interaction. The obtained result is a striking contrast to the early theoretical results [2] and is consistent with the newly observed experiment [1].

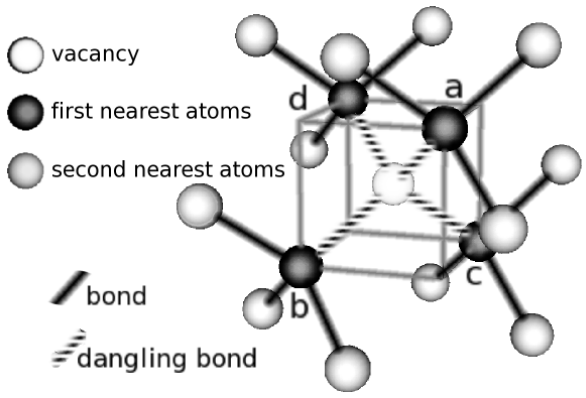

Figure 1: Vacancy in the silicon crystal.

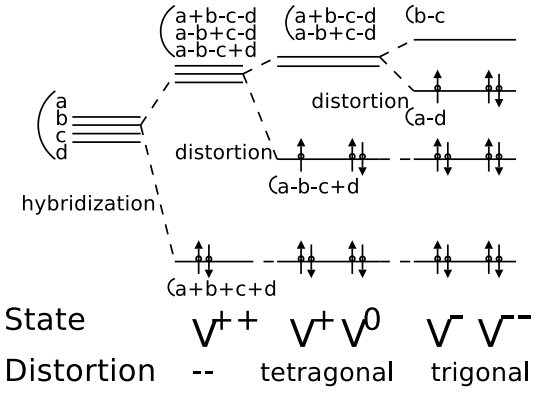

Figure 2: Electronic state at the vacancy site.

[1] T. Goto, H. Yamada-Kaneta, Y. Saito *et al.*, J. Phys. Soc. Jpn. **75** (2006) 044602
[2] G.A. Baraff, E.O. Kane and M. Schlüter, Phys. Rev. B **21** (1980) 5662.